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13. ABSTRACT (Maximum 200 words)

This report summarizes the work performed under two separate two-year programs. Although the research has not concluded, the funding has. Consequently, we discuss the present status of our research, which will proceed to completion despite the unavailability of funds. Our research is concerned with the development of high-performance simulations of non-equilibrium flows in arcjets, with the specific aim of identifying and quantifying frozen flow loss mechanisms and channels. Further details of the research can be found in technical articles cited in this report, as well as in several forthcoming papers.

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RECOVERY OF FROZEN FLOW LOSSES IN ARCJETS

Grant No. AFOSR-91-0318

Final Technical Report

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1.0 INTRODUCTION

Arcjets have proven their space-worthiness with the recent successful launch and operation of two 1.8 KW hydrazine thrusters aboard the AT&T Telstar IV communications satellite in December 1993. Despite this success, there remains a wide margin for improvement in their performance and in fundamental understanding of the loss mechanisms. Arcjets drawing electrical power in the range from 1 KW to 30 KW typically operate at thrust power efficiencies on the order of 30%. The bulk of the remaining 70% is lost in what are known as frozen flow losses. These losses consist of input electrical power expended in dissociation, chemical reaction, ionization, and excitation of internal modes (vibration, rotation, and electronic excitation). It is the aim of this research which has been funded in two 2-year incremental programs (October 1991 - September 1993, and January 1994 - December 1995), to identify and quantify these losses. An additional goal of this research is to explore different ways to recover some of these losses as useful thrust.

Unlike other electric propulsion devices, the arc region of the arcjet is primarily axial near the cathode tip and constrictor regions, and fans out in the radial direction in the supersonic, diverging region of the anode downstream. Thus, the arc is inherently at least two-dimensional. This precludes the use of any analytical models if the important physics of arcjet operation are to be retained. This is the reason that much of the analytical approaches to study arcjet operation to date have largely involved the use of computational tools. Our approach is also computational but differs from its counterpart efforts at MIT, University of Illinois at Urbana-Champaign, Olin Aerospace Corp. (Rocket Research Corp.), and University of Tennessee in several significant ways. First, our approach is the most computationally efficient to date. Second, other approaches utilize adjustable quantities in their formulations without explicitly stating so. Third, our technique allows the modelling of chemical and ionization kinetics on a state-specific, elementary process basis and is scalable to fully 3-D flows. This is the best attainable with current memory constraints on computers.

This report summarizes the research performed under grant no. 91-0318, during the period August 1995 - April 1996. This covers the last half of the second two-year period of our 4-year research program. Unfortunately, at the time of writing of this report, our analysis of the ammonia and hydrazine arcjets have not yet been completed. The tools developed during the course of this research enable us to study these complicated molecular propellants incorporating the electron energy distribution function (EEDF), and we are presently conducting these studies.

1.1 BACKGROUND

Although early tests of arcjet thrusters in the 1960s contributed to the development of a prototype device[1-4], dangerous halting of further development in the 1970s with subsequent revival of space-based defense concepts in the 1980s have led to stagnation in fundamental understanding of the operating characteristics and performance of these devices. In the mid-1980s therefore, the 1 KW and 30 KW designs from the 1960s were revived, tested for lifetime and endurance using ammonia as the propellant, and appeared to meet the mission requirement (Isp~800s) set by the SDIO[5]. However, in 1990, systematic errors were discovered in the thrust measurements made at JPL which led to performance evaluations that failed to meet the mission criteria for the ammonia arcjet. Consequently, all research efforts in the U.S. turned toward the hydrogen arcjet which could easily generate specific impulses on the order of 1500 s. This research was proposed at that time with the following simple argument in mind. Although the ammonia arcjet had an I_{sp} far lower than the hydrogen arcjet, propellant storage and storage cost considerations favor the ammonia arcjet over the hydrogen arcjet. Any gain in I_{sp} in the ammonia arcjet would therefore be a benefit, in addition to the ease of storage and lowering propellant storage costs. Unfortunately, polyatomic propellants such as ammonia usually react to form significant amounts of highly vibrationally excited diatomic species. Thus, a substantial amount of the input electrical energy is lost in frozen flow (i.e. dissociation, ionization, rotational, vibrational, and electronic mode non-equilibrium). Clearly, if these frozen flow losses are to be reduced and if sustained operation is to be achieved at high power levels and high specific impulses, a fundamental understanding of the transport and chemical processes is necessary. Scale-up or scale-down in power is not possible without consideration of the disequilibria between internal and translational modes of molecular motion. It is therefore important to define exactly what is meant by a "non-equilibrium" process.

The words "non-equilibrium" are used in the scientific community to denote a process whose characteristic time scale is comparable to (i.e. neither orders of magnitude larger nor smaller than) the time scale set by a flow. There are in general two time scales in a real flowing fluid. The first is the convective time scale defined as a macroscopic characteristic length divided by a characteristic velocity, and the second is a diffusive time scale defined as the square of a characteristic length divided by the kinematic viscosity. According to classical thermodynamics, a system is in equilibrium if there are no gradients in any properties of the fluid. However,

when there is a flowing compressible fluid, there are gradients in velocity, density, etc. Consequently, one of the "ideal" flows that is commonly used for model comparisons is one that is in local thermodynamic equilibrium. Such an equilibrium flow is one in which the time scales for all processes are infinitely smaller than either the convective or diffusive time scale. A second "ideal" flow is "frozen" flow, which refers to the case where the time scale for a particular process is much longer than the convective or diffusive time scale. Hence, the chemical composition is "frozen" or unchanging.

A given process (i.e. dissociation, ionization, recombination, chemical reaction, etc.) can be out of equilibrium in a flow if the time scale for this process is comparable to the convective time scale. Hence it is possible for flows to consist of many processes, some of which are in local thermodynamic equilibrium, some that are frozen, and others that are out of thermodynamic equilibrium. The processes that are out of equilibrium in this sense are called "non-equilibrium processes". Since classical thermodynamics does not account for the rate at which a process may take place, there is no recourse but to resort to the consideration of rates of processes. Rate processes in chemical kinetics is a term broadly used by many scientists to denote finite-rate reactions (as opposed to infinite rates which correspond to equilibrium conditions, and zero rates which correspond to frozen states). Thus any reaction (especially an elementary process) is described by some rate at which it proceeds. In many applications, reactions are described by overall rates and an overall chemical equation despite the fact that the actual process takes place via several elementary steps or processes.

In reality, chemical processes (dissociation, ionization, recombination, reaction, etc.) proceed at different rates depending on the detailed initial state of the reactants. For atomic reactants this means that the reaction may proceed from a specific electronic configuration or state of the atom. For molecular reactants, the reaction may proceed from specific vibrational and rotational levels in a specific electronic state. The rate of such a process or reaction therefore depends on vibrational quantum number and rotational quantum number for a given electronic state. The kinetic rates for such elementary processes are what are known as "state-specific kinetic rates". There has been a rapid growth in the generation of state-specific rate data for many molecules over the past decade or so, due in part to the sophisticated diagnostics methods that have been devised. The time is therefore ripe to make use of such detailed and accurate information where available, and to combine them with recent rapid advances in supercomputing.

For high speed flows of interest to rocket engines (chemical or electrical), such state-specific information is vital because it determines transport properties (since they are dependent on the chemical composition of the gas mixture), which are continuously changing due to the varying flow field. However, also of vital importance is the fact that when molecular species are present in high speed flows (and this is true of all molecular propellants in supersonic nozzle flows whether it is a chemical or an electrical thruster), a substantial amount of energy can be tied up in

the internal modes (vibration, rotation, electronic). This energy is of no use in generating thrust because it is not in translation motion(i.e. it is not directed kinetic energy). Consequently, energy tied up in these internal modes is "lost", and along with dissociation and ionization, are termed "frozen flow losses". The term "frozen flow losses" is apt because the characteristic relaxation time for the vibrational modes, or rotational modes, or electronic modes are longer than the local convective time scale. Hence, the energy is "frozen" in these modes. This is not to be confused with the "frozen flow" concept addressed earlier which usually refers to non-varying chemical composition.

With the aforementioned definitions and distinctions in mind, the existing literature on arcjet flows can now be reviewed. Several research groups have undertaken study of arcjet flow dynamics both computationally and experimentally. Their work will be reviewed here briefly. Schrade et. al. [6] have modeled two-dimensional, axi-symmetric, fully ionized flow in an MPD arcjet. While this has relevance to the hybrid (electromagnetic/electrothermal) device, it is not directly applicable to the arcjet which is a purely electrothermal device. The main drawback is that the detailed finite rate chemistry which is vital to arcjet performance, is not modeled. Schrade et. al.[7,8] have extended their two-fluid, quasi one-dimensional model in order to study the interaction between the flow in the hot arc and the cooler outer flow in the constrictor region of the arcjet. Their focus has been mainly to understand the arc attachments and arc dynamics in the constrictor region[9]. Butler et. al.[10], King and Butler[11], and Rhodes and Keefer[12] have also modeled of two-temperature axi-symmetric flows in arcjets. A common denominator however in all the aforementioned works is that the state-resolved chemistry (especially including vibrational and electronic non-equilibrium) is neglected. Additionally, many of these investigators are utilizing methods (such as SIMPLE[13], for instance) commonly avoided for viscous supersonic internal flows, on grids that are coarse (less than 50 x 50 for instance). Rhodes and Keefer even mention that when swirl is added to their model, no converged solution could be obtained[12]. Such results. although first in modelling of arcjet flows, should therefore be treated with cautious optimism.

More recently, several research efforts in addition to ours are beginning to produce better simulations of arcjet flows[14-17]. Miller & Martinez-Sanchez have produced the first two-temperature model of hydrogen flow in a 30 KW arcjet geometry[14]. As expected, they predict the state of the gas to be described by a single temperature in the upstream and constrictor regions, while the difference between the electron and heavy particle temperatures becomes acute further downstream in the supersonic, diverging section. While this two-temperature description is likely true and applicable for hydrogen, it will not describe the flows in ammonia or hydrazine arcjets. The same applies to other multi-temperature models of 1 KW hydrogen arcjet flows[15,16]. To date, there exists one reported simulation of ammonia and simulated ammonia arcjets[17]. However, this latter work considers the flow to be in local thermodynamic equilibrium, applies equilibrium chemical

kinetics, and therefore its predicted chemical compositions, and temperatures are highly suspect.

In contrast to existing work described above, the method used in our research is proven to be highly accurate and reliable. Furthermore, our scheme is equally applicable to quasi 1-D, 2-D axi-symmetric, as well as 3-D problems including large sets of master rate equations describing rate processes. The ultimate power of this technique is evident especially when applied on modern supercomputers. The present research therefore represents a significant advance in the state-of-the-art.

2.0 RESEARCH OBJECTIVES

The objectives of this research are:

(1) to study and quantify detailed vibrational and electronic non-equilibrium energy transfer processes in the arcjet nozzle,

(2) to quantify the ro-vibrational populations using modern information on state-resolved rate constants to enable accurate determination of frozen flow losses, and

(3) to numerically study the effects of dilution of the propellant feed with a fast Vibration-Translation (VT) relaxer, on recovery of frozen flow losses.

3.0 STATUS OF RESEARCH EFFORT

The discussion below summarizes the highlights of the research efforts under the third year and early part of the fourth year of this grant. A more detailed discussion can be found in the appendix and references[18-21].

3.1 PROGRESS

The first two years of Grant AFOSR-91-0318 has focused on selection of a numerical scheme that is (1) appropriate for supercomputing, that (2) scales from quasi-1D through 2-D to fully 3-D problems, and which can (3) be easily extended to thousands of states associated with the different species present in the supersonic nozzle of the arcjet. The second two years of this four-year research program were to have been devoted to simulation of the hydrogen, ammonia, and hydrazine arcjets. *However, an unplanned detour in research direction had to be implemented.* Due to the difficulties encountered with solution of Maxwell's equations and suspected improvisations made in existing models[14-17], much of our third year effort was expended in exploring the various ways of modelling the arc attachment in the arcjet. During the third year of this grant, we attempted to solve the magnetic diffusion equation as reported by various authors[14-17]. We found that ad-hoc adjustable parameters were being introduced into the respective models by various means not explicitly mentioned in the literature. These include prescribing point-wise conductivity distributions or not running their simulations for sufficiently long times[15], or specifically blocking out regions near the anode for current

conduction by setting the current density locally to 0[14], or by prescribing the B-field distribution along the anode wall, in effect prescribing the anode attachment[16]. Consequently, **our progress has been retarded**. To date, we have completed simulations of a 30 KW hydrogen arcjet operating at ~ 10 KW power (same as ref.[14]), and a 1 KW hydrogen arcjet to make detailed comparisons with experiment[22]. Work on the 1 KW hydrazine and ammonia thrusters will be completed later this year, despite termination of this grant. Results for the 30 KW hydrogen have been reported in earlier annual technical reports. Here, we present new results on the 1 KW hydrogen arcjet, and comparisons with experimental data obtained at Phillips Laboratory by Jeff Pobst.

Fig. 1 shows a schematic of the 1 KW arcjet geometry, with an exit-to-throat area ratio of 225. Results are shown here for a total current of 10 Amperes, power of 1.4 KW, and mass flow rate of 13.1 mg/s. Figures 2-8 show contours of enclosed current, temperature, dissociation fraction, and exit plane profiles of streamwise component of velocity, temperature, atomic hydrogen concentration, and dissociation fraction, respectively. Also shown in these figures are the experimental values obtained from Pobst at Phillips Laboratories. As can be seen, the agreement between our model predictions and experiment are quite good. The specific impulse was found to be 736 s, and the efficiency was predicted to be 47% (based on thrust power divided by total input power). Approximately 39% of the total power input is found as frozen flow loss at the exit plane. This loss is due to dissociated hydrogen which is unable to recombine into molecular hydrogen before exiting the thruster. The distribution of the total power into various parts of the flow are summarized in the table below:

Summary of distribution of input electrical power	
Total electrical power input (integral of E•j over the internal volume confined by the cathode and anode boundaries)	1,405 W
Frozen flow power lost to dissociation (integral of $n_H w \varepsilon_D$ over the area at the exit plane)	630 W
Thrust power (integral of ρw^2 over the area at the exit plane)	768 W
Translational power loss (integral of $3n_{total}wkT/2$ over the area at the exit plane)	227 W
Frozen flow power lost to ionization (integral of $n_e w \varepsilon_I$ over the area at the exit plane)	< 1 W

From the above table, it can be easily verified that the sum of the power losses and thrust power do not add up to the electrical power into the arcjet. This is because of additional sources of energy generation, particularly viscous dissipation and

numerical artificial dissipation. Nevertheless, it is encouraging that energy is conserved overall to within less than 15%.

As can be seen from Figs. 5-7, the agreement between the present numerical predictions and the experimental results obtained at Phillips laboratories are quite good. There are however some apparent discrepancies, which need to be resolved. First, our numerical simulations underpredict the experimentally measured velocities by as much as 20%. Secondly, our exit plane temperature profile indicates the presence of a prominent bulge (likely due to viscous dissipation and heating due to H-atom recombination). It is uncertain whether this bulge exists in the experimental results because of the scatter. In contrast, agreement between model and experiment is very good in prediction of atomic hydrogen concentrations at the exit plane. The numerical results underpredict the H-atom concentrations by about a factor of 2. This can easily be explained by uncertainty in the known rates, as well as by the existence of another channel for production of H atoms which has been neglected in the results presented here. This additional channel consists of:

$$e^- + H_2 \longrightarrow e^- + e^- + H_2^+,$$

followed by $e^- + H_2^+ \longrightarrow H + H$

The last step (dissociative recombination) is extremely fast and can occur at low pressures since it involves only 2-body collisions.

From the foregoing results, it is evident that the predominant species at the exit plane of this hydrogen arcjet is molecular hydrogen. These are then followed by atomic hydrogen, and hydrogen ions (equal to the electron concentration) respectively. Thus, from the viewpoint of frozen flow losses, it can be seen that a significant amount of energy per molecule of hydrogen propellant is expended in dissociating it is not recovered as useful thrust. Unfortunately, there is no easy means of recovering this energy since recombination of atomic hydrogen to form molecular hydrogen requires many collisions and the exit of the arcjet is usually at a very low pressure ranging from a few torr to several millitorr. It is important to recognize that the situation is different for ammonia and hydrazine propellants, where substantial energy is expected to be stored in vibrational and electronic excitation of molecules such as N_2 at the exit plane. Consequently, while little improvement in hydrogen arcjet performance can be obtained, there is much promise in the improvement of hydrazine and ammonia arcjet performance.

3.2 ON-GOING & FUTURE WORK

At present, we are modeling the arcjet flow in an 800 W hydrogen arcjet. Experimental measurements of exit plane velocity and temperature are being made at the Air Force's Phillips Laboratories[22] and will be supplied to us shortly. We are conducting our simulations and are preparing to conduct comparisons between our model predictions and measurements. To date, we have found that due to the severity of the 1 KW geometry (exit-to-throat area ratio of ~225 versus 25 for the 30 KW geometry), the results are sensitive to the amount of artificial dissipation

present in our simulations in the supersonic region of the flow. We are working on a remedy for this problem, and expect to have it resolved shortly.

Our final task, with the aim of fulfilling our goal of simulating the hydrazine arcjet with state-specific kinetics, is on-going and will be completed by the end of calendar year 1996. Following this last development, we anticipate using these numerical simulations to explore ways of reducing frozen flow losses.

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(20) Babu, V., Aithal, S., and Subramaniam, V. V., "Vibrational Non-equilibrium in arcjet flows", Paper IEPC-93-129, Presented at the 23rd International Electric Propulsion Conference, September 13-17, Seattle, Washington, 1993.

(21) V. Babu, S. Aithal, and V. V. Subramaniam, "On the Effects of Swirl in Arcjet Thruster Flows", paper IEPC-93-183, presented at the 23rd International Electric Propulsion Conference, Seattle, Washington, September 13-17, 1993.

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5.0 PERSONNEL

V. V. Subramaniam	Principal Investigator
V. Babu	Post-doctoral Research Associate, presently Staff Scientist at the Scientific Research Laboratory at Ford Motor Company.
S. M. Aithal	Graduate Research Associate (Ph.D. candidate)
J. Lewis	Graduate Research Associate (M.S./Ph.D. candidate)

6.0 PUBLICATIONS

(1) V. Babu, and V. V. Subramaniam, "Numerical Solutions to Nozzle Flows with Vibrational Nonequilibrium", **J. Thermophysics & Heat Transfer**, Vol. 9, No. 2, pp. 227-232, April-June 1995.

(2) V. Babu, S. M. Aithal, and V. V. Subramaniam, "Numerical Simulation of a Hydrogen Arcjet", submitted to **J. Propulsion & Power** (accepted for publication).

(3) Babu, V., Aithal, S., and Subramaniam, V. V., "Vibrational Non-equilibrium in arcjet flows", Paper IEPC-93-129, Presented at the 23rd International Electric Propulsion Conference, September 13-17, Seattle, Washington, 1993.

(4) V. Babu, S. Aithal, and V. V. Subramaniam, "On the Effects of Swirl in Arcjet Thruster Flows", paper IEPC-93-183, presented at the 23rd International Electric Propulsion Conference, Seattle, Washington, September 13-17, 1993.

(5) S. M. Aithal, V. V. Subramaniam, and V. Babu, "Numerical Simulations of Non-Equilibrium Plasma Flows", Paper 96-2024 **(Invited)** to be presented at the 27th AIAA Fluid Dynamics Meeting, New Orleans, Louisiana, June 18-21, 1996.

(6) S. M. Aithal, V. V. Subramaniam, and V. Babu, "Effects of Arc Attachment on Arcjet Flows", Paper 96-3295 to be presented at the 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Lake Buena Vista, Florida, July 1-3, 1996.

7.0 INTERACTIONS

(1) Dr. Siegfried Jannsen, The Aerospace Corporation.
(2) Prof. W. R. Briley, Mississippi State University.
(3) Prof. Dennis Keefer, University of Tennessee.
(4) Dr. Ingrid Wysong, Phillips Laboratory, Edwards AFB
(5) Dr. Jeffrey Pobst, Phillips Laboratory, Edwards AFB
(6) Dr. David Campbell, Phillips Laboratory, Edwards AFB
(7) Prof. Iain Boyd, Cornell University.

8.0 INVENTIONS & PATENTS

No disclosures have yet been filed, although several ideas for improving arcjet efficiency have been generated.

9.0 HONORS/AWARDS

(1) **1991** **Presidential Young Investigator Award**, National Science Foundation.
(2) **1991** **Award for Excellence in Teaching**, Industrial Advisory Board, Department of Mechanical Engineering, The Ohio State University.
(3) **1992** **Lumley Research Award**, College of Engineering, The Ohio State University.
(4) **1992** **Charles E. MacQuigg Award for Teaching Excellence**, College of Engineering, The Ohio State University.
(5) **1995** **Harrison Award for Excellence in Engineering Education**, College of Engineering, The Ohio State University.
(6) **1996** **Sphinx Senior Honorary Faculty Recognition**, The Ohio State University.

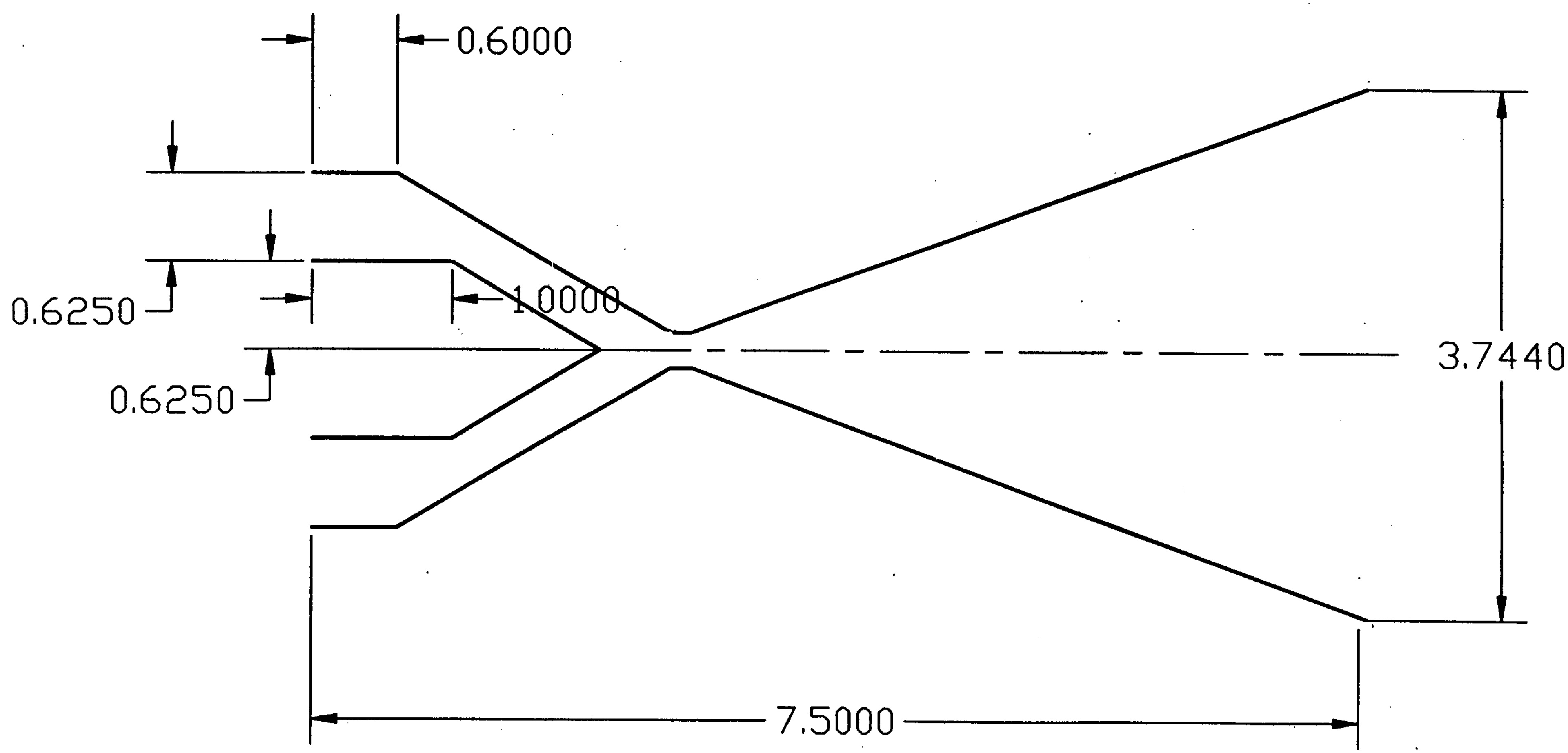

Fig. 1: The 1 KW arcjet geometry, with dimensions non-dimensionalized by 0.1 inches

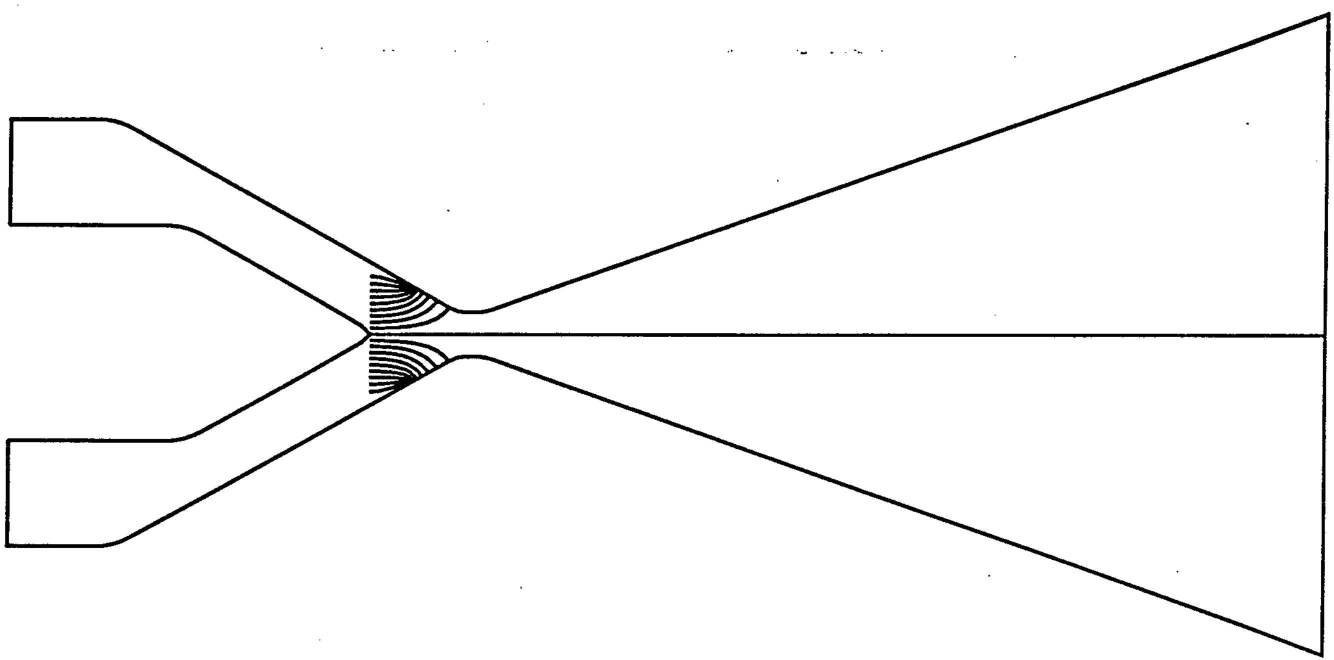

Fig. 2: Contours of enclosed current for the 1.4 KW arcjet operating at 10 A, 13.1 mg/s. The contour values represent actual current values in Amperes.

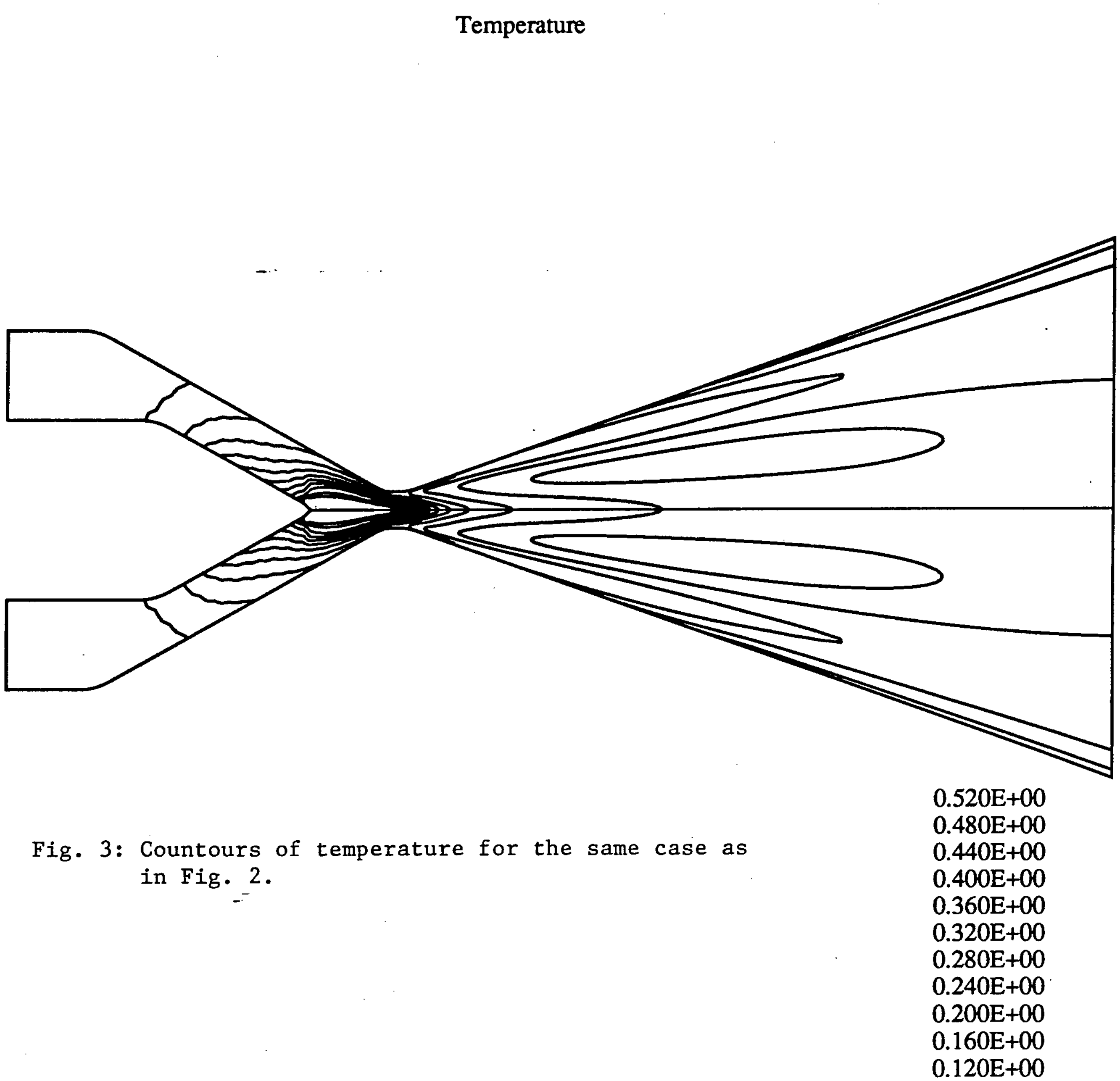

Fig. 3: Countours of temperature for the same case as in Fig. 2.

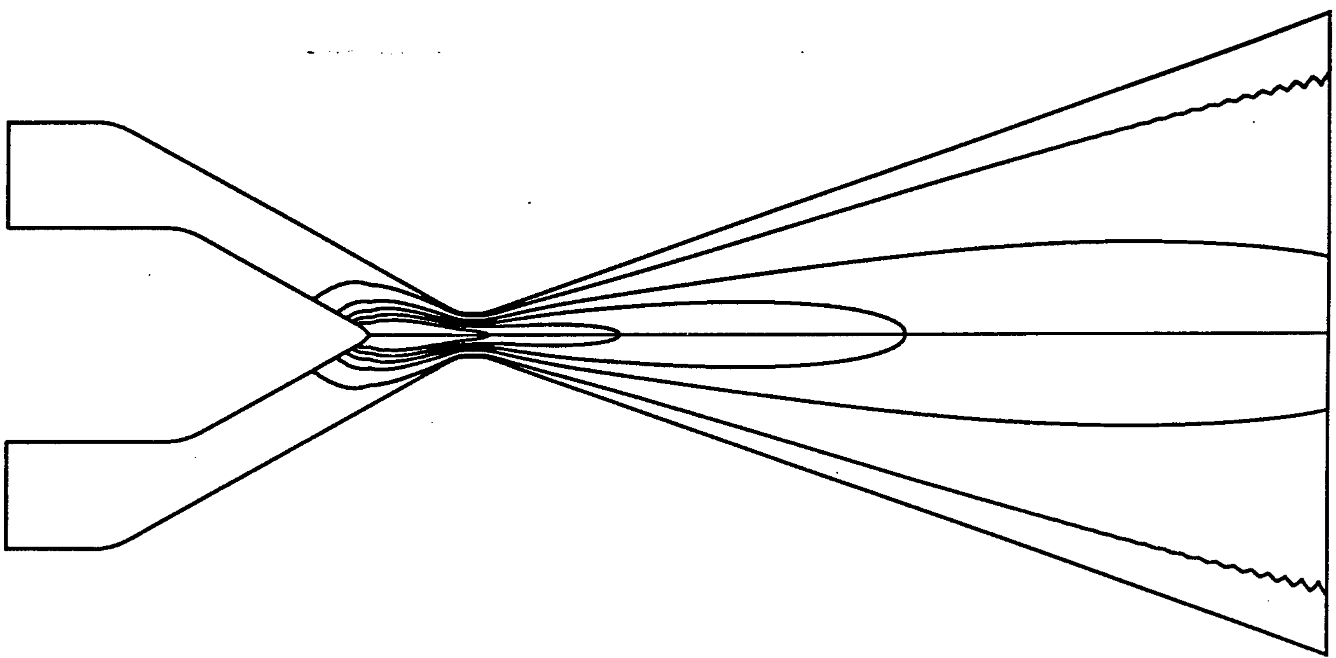

Fig. 3: Countours of dissociation fraction for the same case as in Fig.2. Contour values represent percentages of molecular hydrogen that is dissociated into atomic hydrogen.

UPSTREAM ATTACHMENT

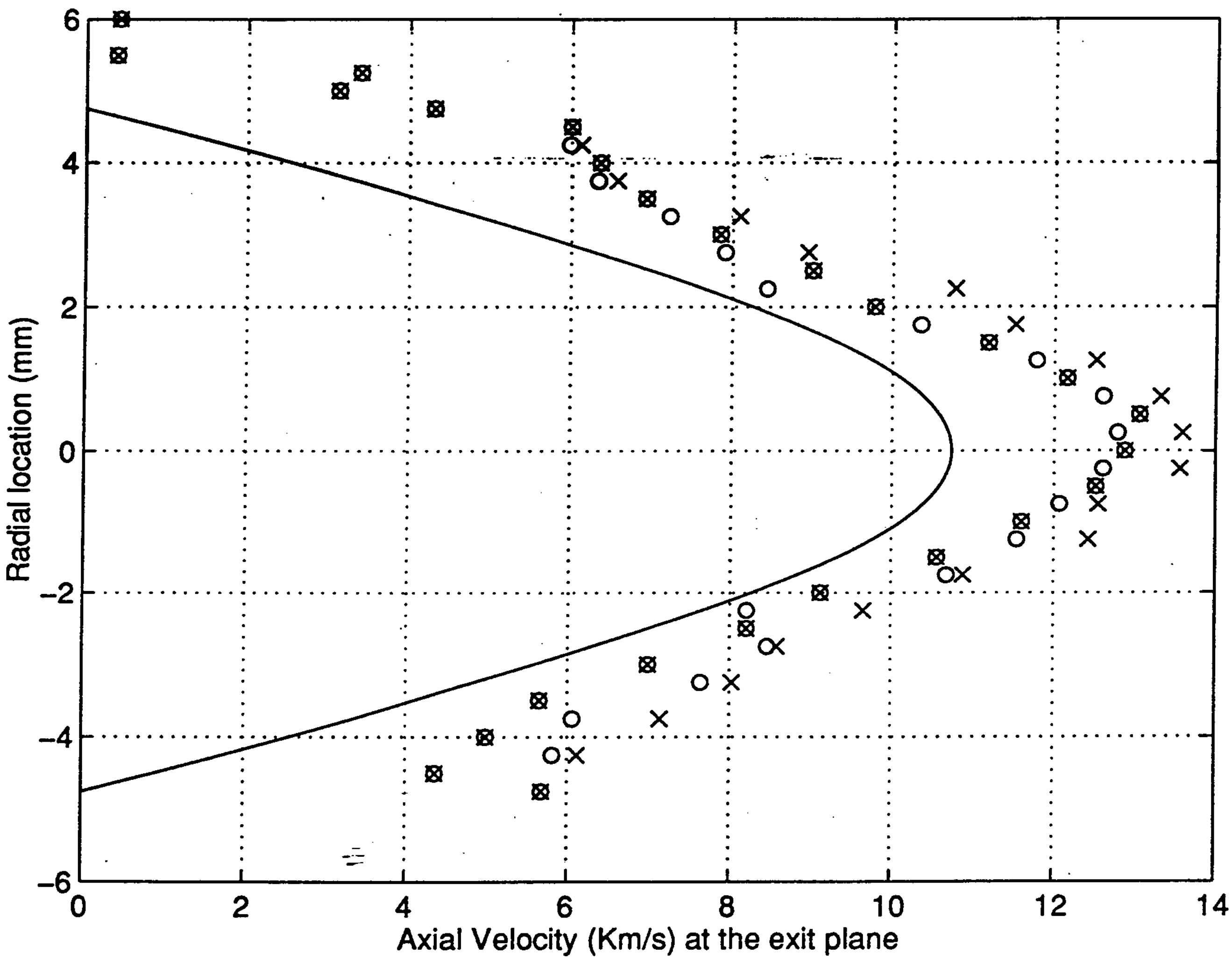

Fig. 5: Comparison between numerical model (solid curve) and experimental data obtained from Phillips Laboratories (Xs indicate maximum measured values while Os indicate minimum measured values. These are plotted for the same case as in Fig. 2.

Upstream Attachment

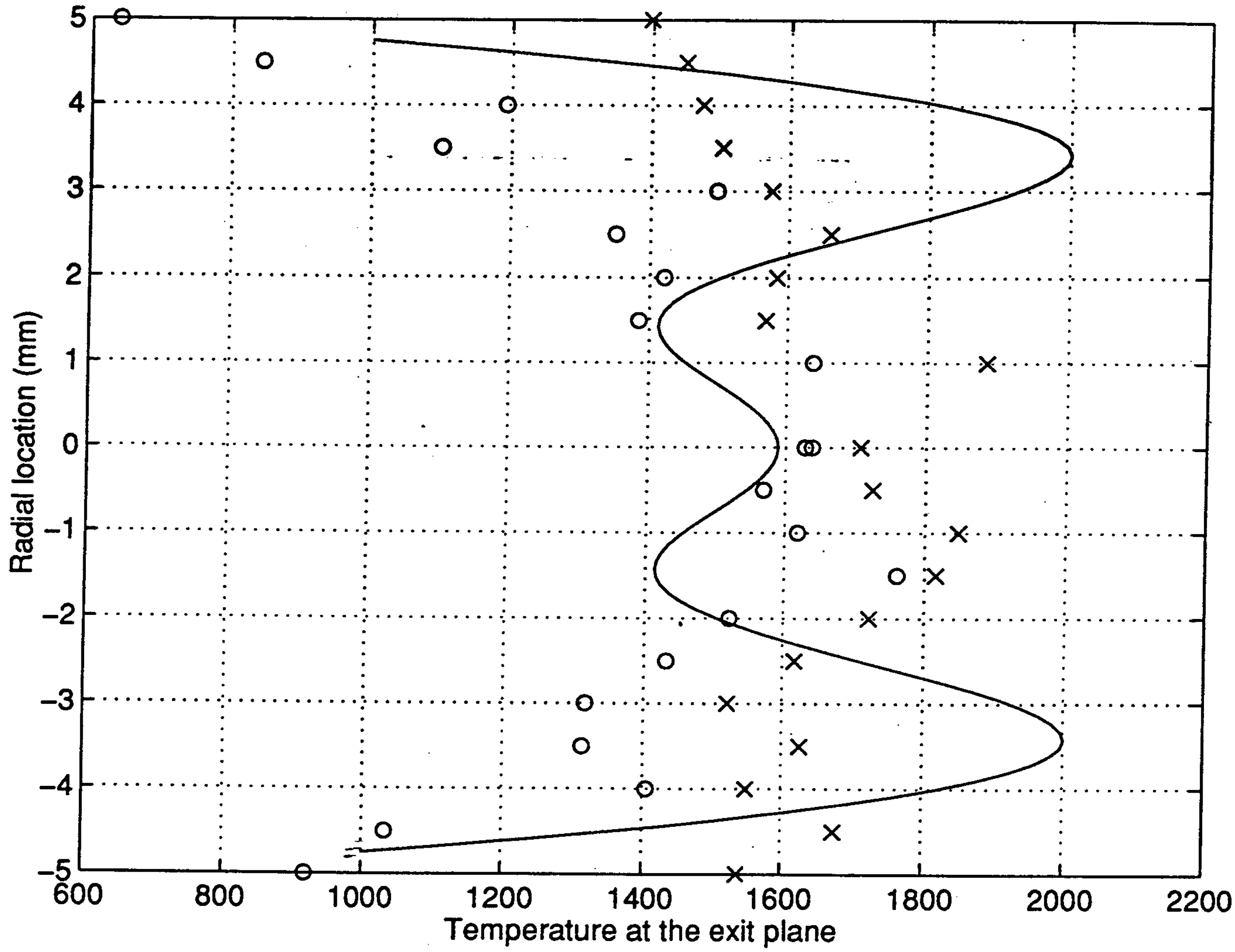

Fig. 6: Comparison of temperature at the exit plane between numerical model and experiments conducted at Phillips Laboratories.

UPSTREAM ATTACHMENT

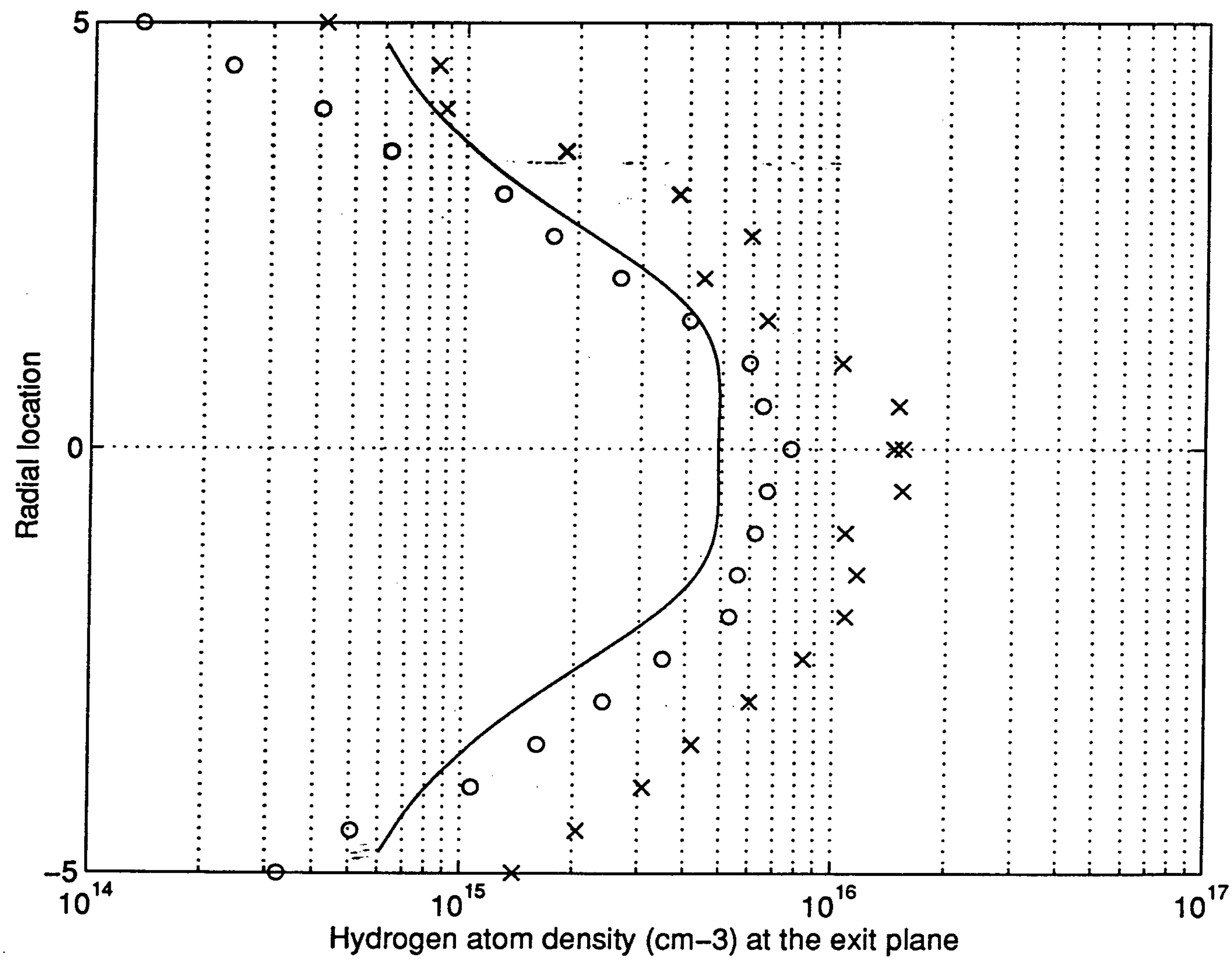

Fig. 7Comparison of atomic hydrogen concentrations at the exit plane between numerical model and experimental results obatined at Phillips Laboratories.

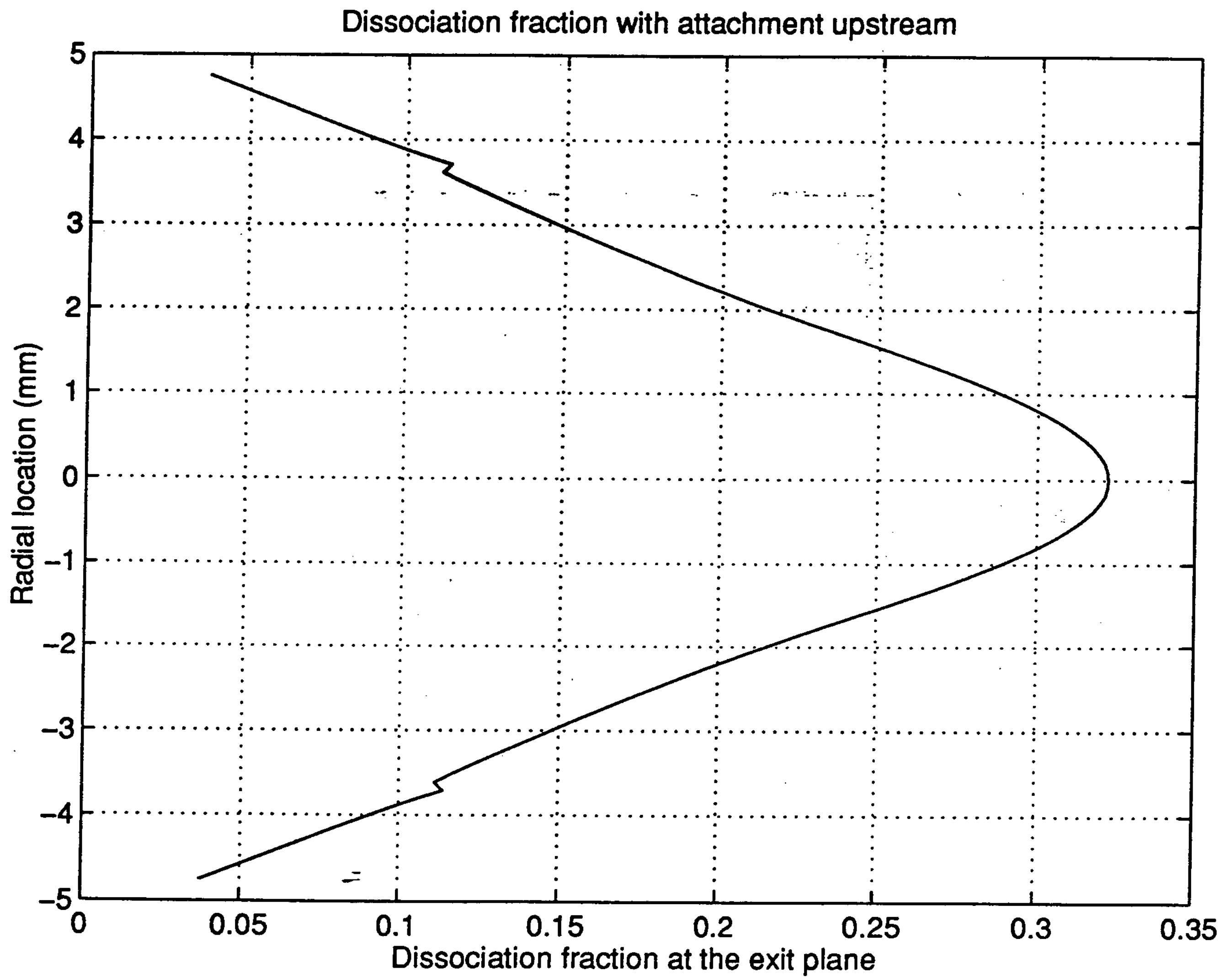

Fig. 8: Radial variation of the dissociation fraction at the exit plane. Our numerical model predicts a maximum value at the centerline of 0.32, while the maximum centerline values measured experimentally were reported to be in the range of 0.45 to 0.5.